

Supplement to Figure 1; (1-S4). Structure refinement statistics for Structures I, II, III, IV, V

Structures	Resolution (FSC=0.143)	Real-space R-factor	RMSD * Bond lengths (Å)	RMSD Angles (°)
I	4.0	0.255	0.017	1.2
II	3.5	0.197	0.014	1.1
III	4.2	0.271	0.02	1.2
IV	4.0	0.235	0.016	1.1
V	3.95	0.225	0.016	1.1

* RMS (root-mean-square) deviations from ideal covalent bond lengths and angles (Engh and Huber, 1991).